Experimental validation of a fuel additive assisted regeneration model in silicon carbide diesel filters

G A Stratakis, G N Pontikakis and A M Stamatelos*
Mechanical and Industrial Engineering Department, University of Thessaly, Volos, Greece

Abstract: In this paper, an experimental validation procedure is applied to an improved one-dimensional model of fuel additive assisted regeneration of a diesel particulate filter. Full-scale tests on an engine bench of the regeneration behaviour of a diesel filter fitted to a modern diesel engine run on catalyst-doped fuel are employed for this purpose. The main objectives of the validation procedure concern the ability of the model to predict the effects of exhaust mass flowrate, initial soot loading mass, volatile organic fraction of the soot and additive concentration in the fuel. The results of the validation procedure are intended to demonstrate the scope and extent of applicability of models of this type to real-world design and optimization studies with diesel filters.

Keywords: diesel engine, diesel particulate filter, mathematical modelling, experimental validation

NOTATION

\( R_g \) universal gas constant = 8.314 J/(mol K)
\( t \) time (s)
\( T/C \) thermocouple fitted on the experimental layout
\( TF \) temperature of filter
\( TGA \) thermogravimetric analysis
\( T \) temperature (K)
\( u_z \) exhaust gas velocity (m/s)
\( VOF \) volatile organic fraction
\( V \) volume (m³)
\( w \) thickness (m)
\( y \) oxygen molar fraction
\( h \) convection coefficient [W/(m² s)]
\( \lambda \) thermal conductivity [W/(m K)]
\( \mu \) viscosity
\( \xi \) total concentration of the catalytic additive in the soot layer (mol/m³)
\( \rho \) density (kg/m³)
\( \psi \) fractional extent of the catalytic additive oxidation

Subscripts

\( g \) gas
\( in \) gas flow through the inlet channel
\( out \) gas flow through the outlet channel
\( p \) particle (soot) layer
\( s \) substrate
\( w \) gas flow through the wall

The MS was received on 26 September 2003 and was accepted after revision for publication on 17 February 2004.

* Corresponding author: Mechanical and Industrial Engineering Department, University of Thessaly, 383-34 Volos, Greece
1 INTRODUCTION

Cellular ceramic diesel filters with catalytic assistance have demonstrated the capacity to drop particulate emissions below 0.01 g/mile, both for passenger cars and for heavy-duty vehicles. Diesel filter applications date back to the 1980s. The most important mode of diesel particulate filter (DPF) operation is the regeneration procedure, where the particulate matter (also referred to as soot) that has accumulated in the filter is burned to avoid filter clogging. The regeneration of heavily loaded filters is followed by a significant reaction heat release, which may endanger the integrity of the filter. To prevent this, catalytic regeneration techniques are employed for lowering of the soot combustion temperature.

A workable catalytic regeneration technique is to dope the fuel with catalytic additives (usually in the form of organometallic compounds). The design of successful catalytic fuel additive assisted trap systems depends on the solution of problems related to filter durability and additive ash accumulation. The appearance of high thermal stresses resulting from temperature gradients during low space velocity regeneration may reduce filter durability [1]. The presence of significant quantities of adsorbed hydrocarbons is thought to have a role in this process. It causes a characteristic behaviour known as erratic regeneration behaviour and observed at low temperatures [2]. Design optimization of filters made by SiC and cordierite is the subject of intensive research by filter manufacturers, because careful exhaust system design and control can significantly improve filter durability. An important aid in this direction is three-dimensional regeneration and stress modelling, combined with experiment. More details on performing this task are presented in reference [3].

In general, catalytic regeneration models of diesel filters are increasingly applied as the core components of design tools. However, different types of model are necessary in the various stages of design. Thus, one-dimensional modelling is very useful in the initial stages of exhaust system design, whereas three-dimensional stress modelling is equally important in component optimization and detailed design.

The requirements posed by the design engineer necessitate the integration of models in the framework of more complete methodologies, which should integrate the following related activities:

(a) model and code development (including preprocessing and post-processing),
(b) code validation,
(c) experiment design and data acquisition,
(d) quality assurance of experimental data,
(e) the model tuning procedure.

In this paper, it is demonstrated how an improved one-dimensional filter regeneration model is validated against full-scale experimental data with the aim of further model and code development. Firstly, the structure and main characteristics of the current status of development of the one-dimensional catalytic regeneration modelling software of LTTE/UTh is presented. Subsequently, the software is subjected to a validation procedure against full-scale tests of the regeneration behaviour of a diesel filter fitted to a modern diesel engine run on catalyst-doped fuel. The main objectives of the validation procedure concern the assessment of the ability of the model to predict the effects of exhaust mass flowrate, initial soot loading mass, volatile organic fraction of the soot and additive concentration in the fuel.

2 MODELLING CATALYTIC DPF REGENERATION

2.1 General

Design optimization of diesel particulate filter systems is increasingly dependent on efficient modelling of the filter regeneration process [4]. The basic tools in this process are one-dimensional models, because of their speed and simplicity, while multidimensional models are employed during the final stages of the design process for the detailed component design.

In principle, a one-dimensional model should be sensitive to the effects of the following parameters:

(a) filter material and filtration characteristics (material density, mean pore size, porosity, permeability);
(b) filter thermophysical properties (specific heat capacity, thermal conductivity, etc.);
(c) filter geometry (cell density, wall thickness, plug length, filter size);
(d) soot deposit filtration characteristics (soot density, permeability);
(e) soot thermophysical properties (specific heat and thermal conductivity);
(f) soot composition (VOF content);
(g) hydrocarbon adsorption/desorption—combustion characteristics;
(h) fuel additive type and concentration in the fuel and soot;
(i) engine operation point (exhaust gas mass flowrate, soot emissions, fuel consumption).

Although a fairly large variety of models has emerged over recent years in the literature, the pioneering work of Bissett and Shadmann [5] remains a valid, mathematically proper and well-documented approach for thermal regeneration modelling that deserves careful study by any newcomer in the field. This work has been adopted and successfully applied in reference [6] to study and experimentally validate high space velocity thermal regeneration events, with a methodology of filter loading assessment by energy balances. It was further extended...
to cover catalytic regeneration [7]. Bissett [8] extended the zero-dimensional, thermal regeneration model of reference [5] to a one-dimensional model, although he missed the significant contribution of gas–wall convection. A one-dimensional version of the catalytic regeneration model of reference [7] was developed in reference [9] and was employed in a successful validation study based on experiments by other researchers [10]. The one-dimensional model formed the basis of software [11] that is currently employed in diesel exhaust systems design by the automotive and diesel filter industry.

There are two aspects in diesel filter modelling that greatly challenge the accuracy and predictive ability of models:

1. The first is the modelling of filter back pressure which is important for correct assessment of soot loading [12].
2. The second aspect is the study of the kinetic scheme and parameters of catalytic soot oxidation, also addressing adsorbed hydrocarbon oxidation.

A main difficulty encountered in the validation of diesel filter regeneration models, especially as regards the filter back pressure prediction, lies in the extraction of realistic particulate properties by the experiments. Tests with full-scale filters loaded and regenerated under real-world operating conditions are more realistic than those with miniscale filters and synthetic soot accumulation, although the operating conditions (particulate loading, ash accumulation, exhaust mass flowrate, exhaust gas properties) are more difficult to control. For this reason, model validation in this paper is based on the simulation of standardized, full-scale filter regeneration experiments under various scenarios with varying soot loading, VOF content and fuel additive concentration in the fuel.

Together with the pressure drop calculation, the reaction kinetic scheme and kinetic parameters form the core of every diesel filter regeneration model. Nevertheless, out of the numerous cited literature on diesel filter modelling, only a few studies employ an inclusive reaction scheme that introduces all the necessary degrees of freedom in order to model real-world filter operation. This is a severe drawback, especially when dealing with the complex problem of fuel additive assisted regeneration at low temperatures. Therefore, the model presented in this paper includes a reaction scheme that accounts for catalytic chemical reactions, and its validation process focuses especially on the reaction kinetics.

As already mentioned, the improved one-dimensional model developed here is considered as a basic design tool employed in the initial design stage of the DPF to carry out kinetic and pressure drop parameter estimation and to perform parametric optimization tasks. For subsequent detailed design of components, other tools such as three-dimensional stress modelling and computational fluid dynamics (CFD) modelling come to the foreground.

2.2 Geometry of the channels and the soot layer

The DPF consists of a ceramic grid of parallel channels. Adjacent channels are alternatively plugged at each end in order to force the diesel aerosol through the porous substrate walls which act as a mechanical filter. Thus, diesel particulate matter is deposited on the four sides of the inlet channels.

Because of the repeating geometry of the DPF, mathematical treatment may be restricted to a fundamental channel volume of the trap. It is convenient to define it as in Fig. 1. That is, this fundamental volume consists of one inlet channel and four quarters of the four adjacent outlet channels. The boundaries of the volume are assumed to be adiabatic, and no flow occurs through them to the rest of the outlet channel. From the standpoint of modelling, the whole trap is constructed by repeating this fundamental volume.

To formulate the balance equations pertinent for regeneration modelling, a small part of this fundamental volume, of length $\Delta z$, is considered. At this part of the channel, a layer of soot of mass $m$ and thickness $w$ has already accumulated. The wall thickness is $ws$, and the length of the channel edge is $l$. Exhaust gas flow is perpendicular to the soot layer and wall. Exhaust gas species are consumed or produced as gas flows through the soot layer. In this work, subscript ‘p’ will be used to denote the physical properties of the soot layer, and subscript ‘s’ to denote the corresponding properties of the wall.

It is evident from Fig. 2 that the soot layer consists of four trapezoids. In earlier work [9] the trapezoids were approximated as rectangles, but the approximation yields considerable error regarding the soot layer thickness, especially for highly loaded filters. The layer thickness

![Fig. 1](image-url) Fundamental volume of a wall flow diesel particulate filter consisting of one inlet channel and four adjacent outlet channels
calculation is important, especially in the calculation of the model back pressure. Therefore, in this work, the exact description of the soot layer geometry is introduced. Assuming that some soot mass $m$ of density $\rho_p$ is deposited on a filter channel with inner side length $\ell$, the deposit thickness can be calculated as

$$w = \frac{1}{2} \left( \ell - \sqrt{\ell^2 - \frac{m}{\rho_p \Delta z}} \right)$$

(1)

This relation is used by the model to compute the thickness of the deposit, which, in turn, is needed for calculation of the filter pressure drop and flowfield distribution. As a consequence of the trapezoidal distribution of the soot layer, the area perpendicular to the flow $A(x)$ (i.e. the area that the flow ‘faces’ at each $x$) also changes along $x$:

$$A(x) = \begin{cases} 
4(2x + \ell)\Delta z, & -w \leq x \leq 0 \\
4\ell \Delta z, & 0 \leq x \leq w_s 
\end{cases}$$

(2)

The volume of the soot layer may be readily calculated from the above relationship

$$V_p = 4\Delta z(l - w)w$$

(3)

### 2.3 Reaction kinetics

The soot that is deposited in the DPF walls consists mainly of carbon and adsorbed hydrocarbons [also known as volatile organic fraction (VOF)]. When a fuel additive is used to assist regeneration, additive is present in the formation process of the particles in the combustion chamber of the engine. Therefore, the soot particles that are deposited in the trap contain bound metal oxide particles. These particles react with the carbon and VOF of the soot at much lower temperatures compared with those needed for oxygen.

The kinetic model that will be described here accounts for catalytic combustion of soot owing to a Ce-based fuel additive, but does not include the effect for the VOF. The model for catalytic oxidation of carbon was first formulated by Koltsakis and Stamatelos [6]. The implemented mechanism is only valid when the catalytic oxide has two oxidation states, which is true for ceria. When ceria is in a low oxidation state, it can form a trivalent Ce oxide (Ce$\text{O}_3$); when it is in a high oxidation state, it can form a tetravalent Ce oxide (Ce$\text{O}_4$). The first step of the mechanism is oxidation of Ce$\text{O}_3$ by O$_2$ to produce Ce$\text{O}_2$. The second step involves reaction of Ce$\text{O}_2$ with soot carbon. Ceria returns to its trivalent state while carbon monoxide is produced. The presence of additive does not prevent the direct oxidation of carbon by oxygen if the temperature is sufficient for this reaction. The reactions are given, along with their reaction rates, in Table 1.

The reaction rates for all reactions are assumed to follow first-order Arrhenius-type expressions. For thermal carbon oxidation and Ce$\text{O}_3$ oxidation the rate is proportional to the oxygen concentration in the exhaust gas. In the two reactions of catalyst-assisted regeneration, the quantity $\psi$ is employed. Here, $\psi$ represents the mole percentage of Ce in its higher oxidation state Ce$\text{O}_2$

$$\psi = \frac{\text{mol CeO}_2}{\text{mol Ce}} = \frac{\text{mol CeO}_2}{2 \text{ mol Ce}_2\text{O}_3 + \text{mol CeO}_2}$$

(4)

The quantity $\xi$ will also be needed in this study. It is defined as the concentration of catalyst in the soot layer and is a function of the metal additive concentration in the fuel. It may be expressed as

$$\xi = \frac{\text{mol Ce}}{\text{mol soot}} = \frac{2 \text{ mol Ce}_2\text{O}_3 + \text{mol CeO}_2}{\text{mol C}}$$

(5)

It should be noted that both $\psi$ and $\xi$ are viewed as averaged quantities through the soot layer thickness.

### 2.4 Mass and heat balances (regeneration submodel)

As gas flows through the soot layer, the oxygen is gradually depleted because of reaction with carbon and ceria. An oxygen concentration profile is thus established through the soot layer, which is expressed by an oxygen mass balance

$$\frac{m_p}{A(x)} \frac{dy}{dx} = -M_y[k_1 + 0.5k_2 + 0.5k_3(1 - \psi)]y$$

(6)

### Table 1 Reaction and rate expressions of the regeneration model

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Rate expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. $C + O_2 \rightarrow CO_2$</td>
<td>$r_1 = k_1 y$</td>
</tr>
<tr>
<td>2. $C + 0.5O_2 \rightarrow CO$</td>
<td>$r_2 = k_2 y$</td>
</tr>
<tr>
<td>3. $C + 4CeO_2 \rightarrow 2CeO_3 + CO_2$</td>
<td>$r_3 = k_3 \psi$</td>
</tr>
<tr>
<td>4. $C + 2CeO_2 \rightarrow Ce_2O_3 + CO$</td>
<td>$r_4 = k_4 \psi$</td>
</tr>
<tr>
<td>5. $Ce_2O_3 + 0.5SO_2 \rightarrow 2CeO_2$</td>
<td>$r_5 = k_5(1 - \psi)$</td>
</tr>
</tbody>
</table>

$k_i = A_i e^{-E/RgT}, \quad i = 1, \ldots, 5.$
The above mass balance may be solved to obtain the oxygen concentration profile \( y(x) \), for the initial condition \( y(x = -w) = y_{in} \), provided that the temperature is considered uniform through the soot layer. This is a fundamental assumption that is supported by the original work of Bissett and Shadmann [5] (see also the boundary conditions below). The solution yields the total consumption of oxygen \( \Delta y = y(x = -w) - y(x = 0) \) through the soot layer

\[
\Delta y = y_{in} \left[ 1 - \exp \left( -\frac{M_g[k_1 + 0.5k_2 + 0.5k_3(1 - \psi)]}{m_g} \right) \right] V_1
\]  

(7)

The total consumption of oxygen may be used to calculate the rate of soot consumption because of both thermal oxidation with oxygen and catalytic oxidation with ceria. Specifically, the mass balance for the soot mass consumption is

\[
\frac{\rho_p}{M_C} \frac{dV_p}{dt} = - \int_{-w_p}^{0} \left[ (k_1 + k_2)y + (k_3 + k_4)\psi \right] A(x) \, dx
\]

(8)

or, splitting the integral

\[
\frac{\rho_p}{M_C} \frac{dV_p}{dt} = -(k_1 + k_2) \int_{-w_p}^{0} y A(x) \, dx
\]

(9)

The first integral contained in the right-hand side of the above equation may be calculated from the oxygen mass balance (6)

\[
\int_{-w_p}^{0} y A(x) \, dx = \frac{m_g}{M_g[k_1 + 0.5k_2 + 0.5k_3(1 - \psi)]} \Delta y
\]

(10)

The second integral of the soot mass balance is the volume of the soot layer, \( V_p \). Substituting the above yields the following rate of soot mass consumption

\[
\frac{dV}{dt} = \frac{M_C}{M_g} \frac{k_1 + k_2}{k_1 + 0.5k_2 + 0.5k_3(1 - \psi)} m_g V_p
\]

(11)

A mass balance must also be formulated for \( \psi \), which expresses the continuous transition of the catalytic additive between the CeO\(_2\) and Ce\(_2\)O\(_3\) states. According to the CeO\(_2\) mass balance, the rate of change depends on the additive oxidation and reduction reactions, i.e.

\[
\left( \int_{-w_p}^{0} \frac{\rho_p A(x) \, dx}{M_C} \right) \frac{d\psi}{dt} = \int_{-w_p}^{0} \left[ -(4k_3 + 2k_4)\psi + k_3 y(1 - \psi) \right] A(x) \, dx
\]

(12)
released (a) by chemical reactions and (b) by convection because of flow normal to the soot layer and wall
\[
\frac{dQ}{dr} = (\rho_p c_{p,p} V_p + \rho_s c_{p,s} V_s)
\]
\[
= -\left(\Delta H_1 k_1 + \Delta H_2 k_2\right) \frac{m_g \Delta T}{k_1 + 0.5k_2 + 0.5k_3(1 - \psi)} M_g
\]
\[
- (\Delta H_3 k_3 + \Delta H_4 k_4) \psi V_p + \dot{m}_g c_{p,g}(T - \bar{T}_g)
\]  
(16)

2.5 Pressure drop submodel

The total pressure drop across the particulate layer and the ceramic wall can be expressed as the sum of the porous ceramic substrate pressure drop and the soot layer pressure drop
\[
\Delta p = \Delta p_s + \Delta p_p
\]  
(17)

It is generally accepted [13] that the pressure drop associated with flow through ceramic filters can be approximated by Darcy’s law. According to this law, the total pressure drop due to flow through the ceramic wall and the soot layer can be approximated by the following simplified relation
\[
\Delta p = p_{in} - p_{out} = \frac{\mu u_w w_s}{k_s} + \frac{\mu u_w w_p}{k_p}
\]  
(18)

By using the concept of effective particulate layer thickness [14], the latter formula can be rewritten as follows
\[
\Delta p = p_{in} - p_{out} = \frac{\mu u_w w_s}{k_s} + \frac{\mu u_w m_p}{A_k(p k)_p}
\]  
(19)

This formula allows, in principle, the backward approximate calculation of collected soot mass as a function of measured filter back pressure at a certain engine and filter loading operation point, once an approximate value for the product \((p k)_p\), that is, soot layer density times soot layer permeability, is known for the specific engine–filter–operation point combination.

2.6 One-dimensional modelling extension

The above pressure drop and regeneration model is a zero-dimensional approach to filter modelling, in the sense that it is valid for each point \(z\) along the filter axis but does not provide any information regarding axial profiles of temperature, pressure drop and mass distribution. This is accomplished below, employing the following balance equations:

(a) the conservation of the exhaust gas mass flow,
(b) the conservation of the axial component of momentum of exhaust gas,
(c) the conservation of the energy of the exhaust gas,
(d) the conservation of energy for the channel wall.

Below, subscript ‘in’ will be used for the flow parallel to the inlet channel, subscript ‘out’ for the flow parallel to the outlet channel and subscript ‘w’ for flow through the soot layer and the wall.

The exhaust gas mass balances state that, at each axial point of the inlet channel, the change in exhaust gas flow is equal to the flow leaving the inlet channel via the porous wall. An exactly analogous balance is defined for the outlet channel
\[
\frac{\partial}{\partial z}(\rho_{in} u_{in}) = -\left(\frac{4}{7}\right)\rho_u u_w, \quad \frac{\partial}{\partial z}(\rho_{out} u_{out}) = +\left(\frac{4}{7}\right)\rho_u u_w
\]  
(20)

The balance equation for the axial component of the momentum of the gas indicates that the axial pressure variation is due to convective transport of the \(z\) component of momentum and the viscous drag forces exerted in the gas flow. The balance equation is the same for both channels
\[
\frac{\partial p}{\partial z} + \frac{\partial}{\partial z} (\rho_i u_i^2) = -\frac{\partial u}{\partial z}, \quad i = \text{in, out}
\]  
(21)

Viscous drag is caused by the gradient of the axial velocity of the gas, which reduces to zero at the walls. According to Bissett and Shadmann, these drag forces should be similar to those observed for an impermeable wall, because only a small fraction of the gas penetrates the wall at each axial point.

The above balances, together with the Darcy correlation (19), are used to calculate the distribution of the gas velocities in the inlet and outlet channels and the velocities normal to the soot layer and wall. Once the velocity distribution has been calculated, the model computes the energy exchanged between the gaseous and solid-phase porous wall. The energy balances for the inlet and outlet channels are
\[
c_{p,g} \frac{\partial}{\partial z} (\rho_{in} u_{in} T_{in}) = -\left(\frac{4}{7}\right)\rho_u u_w T_{in} + h_{in} \left(\frac{4}{7}\right)(T - T_{in})
\]
\[
c_{p,g} \frac{\partial}{\partial z} (\rho_{out} u_{out} T_{out})
\]
\[
= -\left(\frac{4}{7}\right)\rho_u u_w T_{out} + h_{out} \left(\frac{4}{7}\right)(T - T_{out})
\]  
(22)

The balance for the outlet channel differs in the second term which concerns energy transport via the flow through the porous wall. Apart from the sign of the term, the temperature is different, because the gas leaving the porous wall has the temperature of the wall.

Finally, the axial temperature distribution along the wall is calculated. The heat balance implements
one-dimensional heat conduction, and source terms simultaneously at the inlet and the exit of the filter, and are because of gas–solid heat convection and reaction exothermy

\[ \rho_s c_{ps} + \rho_p c_{pp} \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial z^2} + h_{in} \left( \frac{4}{\ell} \right) (T - T_{in}) + h_{out} \left( \frac{4}{\ell} \right) (T - T_{out}) + \frac{dQ}{dt} \]  

(23)

In the above equation, the heat source term \( \frac{dQ}{dt} \) expresses heat exchange due to perpendicular gas flow and reaction exothermy; it is given by equation (16).

3 DESIGN OF THE VALIDATION EXPERIMENTS

The validation was based on the results of engine bench regeneration experiments performed on an engine bench of the Laboratory of Thermodynamics and Thermal Engines (LTTE). The filter employed in these experiments was a SiC 200 cells/\( \text{in}^2 \) filter (diameter \( \times \) length = 5.66\( \times \)6\( \times \)) fitted in the exhaust pipe of a 2 l displacement HDI turbocharged passenger car engine about 600 mm after turbo. The engine and diesel filter specifications are presented in Table 2. The temperatures were measured simultaneously at the inlet and the exit of the filter, and inside the filter, along a filter diameter 15 mm deep from the filter exit. The exhaust emissions of CO, CO\(_2\), NO\(_x\), and HC were measured simultaneously before and after the filter. The O\(_2\) concentration was calculated by the air–fuel (A/F) ratio obtained from the UEGO sensor installed before the filter inlet. The experimental layout of the filter loading–regeneration experiments is presented in Fig. 3.

The capacity of the model to address the effect of the following design and operation parameters was validated:

(a) fuel additive concentration,
(b) initial filter soot loading,
(c) collected soot characteristics (VOF content \([15]\), etc.),
(d) indirectly, also the effect of the exhaust gas mass flowrate.

The effect of fuel additive concentration on the regeneration was checked at a characteristic medium operation point of 2250 r/min, 60 N m for the catalytic regeneration, employing as reference for the thermal regeneration the non-catalytic regeneration. The effects of 0, 25 and 50 ppm cerium fuel additive concentrations in the fuel were studied. The non-catalytic regeneration was performed at an increased engine speed and load point of 3800 r/min, 60 N m in order to meet the high exhaust temperature levels that are necessary for the initiation of regular soot oxidation. The filter was previously loaded at the medium point of 3000 r/min, 40 N m until a medium soot mass loading of the order of 6 g/l filter was obtained. The shift to a set of experiments with different fuel additive concentrations was performed after filter cleaning and engine running for about 6 h to prevent possible memory effects to the fuel and soot composition. Steady state loading experiments at specific combinations of engine speed and load were

<table>
<thead>
<tr>
<th>Table 2 Engine technical data and diesel filter specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine type</td>
</tr>
<tr>
<td>Cylinders</td>
</tr>
<tr>
<td>Displacement</td>
</tr>
<tr>
<td>Rated power/speed</td>
</tr>
<tr>
<td>Rated torque/speed</td>
</tr>
<tr>
<td>Filter type</td>
</tr>
<tr>
<td>Filter diameter ( \times ) length</td>
</tr>
<tr>
<td>Cell pitch</td>
</tr>
<tr>
<td>Filter wall thickness</td>
</tr>
</tbody>
</table>

Fig. 3 Experimental layout. The engine and digitally controlled dynamometer installation is shown along with exhaust gas analysers, main filter measurement lines and data acquisition system.
performed in order to validate the ability of the model to predict the effect of initial soot loading and VOF content.

Indirect assessment of the effect of the soot deposit filtration characteristics and soot oxidation kinetics was based on variation of initial soot loading (3, 6 and 9 g/l filter), obtained by adjusting the filter loading process duration, assuming constant particulate emissions and no effects of the increased back pressure on the engine exhaust mass flowrate. The filter loading was performed with the engine running on 3000 r/min, 40 N m with 25 ppm cerium doped fuel.

Two characteristic engine operation points were selected for the assessment of differences in the VOF content of soot: 3000 r/min, 40 N m (10 per cent VOF) versus 1800 r/min, 90 N m (2 per cent VOF). These points are characterized by equivalent total particulate matter emissions and cover the range of filter wall temperatures from 300 to 400 °C that is responsible for VOF variation [15]. Secondary effects due to the dynamic phenomena of adsorption–desorption may also affect soot oxidation kinetics.

The engine operation points for the regeneration experiments were specially selected for assessment of the effect of exhaust gas flowrate. The exhaust gas flowrate was varied through the combination of engine speeds of 1500, 2250, 3000 and 4000 r/min with engine loads of 80, 60, 60 and 30 N m respectively, in order to obtain during the regeneration approximately equivalent filter inlet temperature levels in the range 500–550 °C. These points result in a variation in exhaust gas mass flowrate in the range 28–100 g/s and represent the real conditions met under city and extra-urban driving conditions. The appearance of secondary effects related to flow mal-distribution phenomena affected by the flowrate during regeneration is expected to play a significant role in the simulation results [16]. Each regeneration process was initiated after loading at the respective engine operation point, until the same level of filter loading was achieved (6 g/l filter) by a combined step variation in engine load and engine intake airflow obtained with adjustment of the turbocharger and EGR valves. The engine was left to run for 10 min under steady state conditions before the regeneration strategy was applied, a period considered long enough for thermal and chemical equilibrium to be reached.

The experimental protocol is summarized in Table 3. The regeneration experiments were performed in combination with TGA experiments of soot samples taken directly from the filter loaded at the above operation points in order to improve our understanding of the kinetics of soot oxidation by ceria and exhaust gas [17]. Previous experimental work on determination of pressure drop parameters as functions of collected soot mass [12] was employed to support pressure drop parameter selection.

4 VALIDATION RESULTS

Before carrying out the main validation process, it is necessary to determine reference values for pressure drop and kinetic parameters. The source for this information was previous experimental work by the present authors on pressure drop and soot oxidation kinetics, along with published results of experimental work of other researchers.

Starting from the pressure drop parameters, the product of soot permeability times soot density, \((p_k)_p\), is fitted to the experimental behaviour. Experimental determination of these values by dedicated experiments has been attempted in the past by several researchers, but general agreement has yet to be reached [12, 18]. As shown in Table 4, a constant, typical value of \((p_k)_p = 2.25 \times 10^{-13}\) proved successful in most simulations.

Table 3 Experimental protocol

<table>
<thead>
<tr>
<th>Name of studying parameter</th>
<th>Experimental parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ce concentration (ppm)</td>
</tr>
<tr>
<td>Catalyst concentration</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>25*</td>
</tr>
<tr>
<td></td>
<td>50</td>
</tr>
<tr>
<td>Soot mass loading</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td>25*</td>
</tr>
<tr>
<td></td>
<td>9</td>
</tr>
<tr>
<td>Filter accumulation condition</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td>25</td>
</tr>
<tr>
<td>Filter regeneration condition</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Reference experiment.
### Table 4  
CATWALL one-dimensional validation results based on Laboratory of Thermodynamics and Thermal Engines experimental data

<table>
<thead>
<tr>
<th>Name of studying parameter</th>
<th>Value of studying parameter</th>
<th>Soot mass oxidized (grams measured)</th>
<th>CO/CO₂ (experimental)</th>
<th>Wall permeability (m²)</th>
<th>Soot density (kg/m³)</th>
<th>Kinetic parameters</th>
<th>Thermal soot oxidation</th>
<th>Catalytic soot oxidation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalyst concentration (ppm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Aₙ (mol/m²s) E₁ (J/mol) E₂ (mol/m³s) E₃ (J/mol)</td>
<td>Aₙ (mol/m²s) E₁ (J/mol) E₂ (mol/m³s) E₃ (J/mol)</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td></td>
<td>20.5</td>
<td>0.02</td>
<td>2E-13</td>
<td>2.8E-13</td>
<td>80</td>
<td>1E13</td>
<td>1.9E5</td>
</tr>
<tr>
<td>25</td>
<td></td>
<td>14.2</td>
<td>0.14</td>
<td>2E-13</td>
<td>2.8E-13</td>
<td>80</td>
<td>1E13</td>
<td>1.9E5</td>
</tr>
<tr>
<td>50</td>
<td></td>
<td>13.15</td>
<td>0.15</td>
<td>2E-13</td>
<td>2.8E-13</td>
<td>80</td>
<td>1E13</td>
<td>1.9E5</td>
</tr>
<tr>
<td>Soot mass loading (g/l)</td>
<td></td>
<td>8</td>
<td>0.01</td>
<td>2E-13</td>
<td>2.8E-13</td>
<td>80</td>
<td>1E13</td>
<td>1.9E5</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>14.2</td>
<td>0.02</td>
<td>2E-13</td>
<td>2.8E-13</td>
<td>80</td>
<td>1E13</td>
<td>1.9E5</td>
</tr>
<tr>
<td>9</td>
<td></td>
<td>20.5</td>
<td>0.19</td>
<td>2E-13</td>
<td>2.8E-13</td>
<td>80</td>
<td>1E13</td>
<td>1.9E5</td>
</tr>
<tr>
<td>Filter accumulation condition (r/min × N m)</td>
<td>3000 × 40 (VOF 10%) 1800 × 90 (VOF 2%)</td>
<td>14.2</td>
<td>0.14</td>
<td>2E-13</td>
<td>2.8E-13</td>
<td>80</td>
<td>1E13</td>
<td>1.9E5</td>
</tr>
<tr>
<td>Filter regeneration condition (r/min × N m)</td>
<td>1500 × 80 (MFR 28 g/s) 2200 × 60 (MFR 52 g/s) 3000 × 60 (MFR 70 g/s) 4000 × 30 (MFR 92 g/s)</td>
<td>14.2</td>
<td>0.07</td>
<td>2E-13</td>
<td>2.8E-13</td>
<td>80</td>
<td>1E13</td>
<td>1.9E5</td>
</tr>
</tbody>
</table>

Note: Additional columns for pressure drop parameters such as kinetic parameters, thermal soot oxidation, and catalytic soot oxidation are included for a comprehensive analysis.
As regards the wall permeability, a constant value of the order of $2 \times 10^{-13}$ was found to be capable of matching the pressure drop curves of the whole range of validation experiments. This value is in accordance with those reported by other researchers [13]. A summary of the validation runs and the respective kinetic parameter values inserted in the model is presented in Table 4.

The baseline for the determination of $E$ for thermal and catalytic regeneration has been extensive TGA analysis experiments of soot samples taken directly from the filter [17]. The following values for activation energy were determined from the above-mentioned experimental work (Fig. 4):

1. $E = 190$ kJ/mol for complete thermal soot oxidation to CO$_2$, and $E = 150$ kJ/mol for incomplete thermal soot oxidation to CO. In the literature the published values of activation energy of uncatalysed soot oxidation are found to cover a range between 140 and 210 kJ/mol [19–22].

2. $E = 120$ kJ/mol for complete catalytic soot oxidation to CO$_2$, and $E = 80$ kJ/mol for incomplete catalytic soot oxidation to CO. These values agree with the results reported by Summers et al. [23] and Lahaye et al. [24] who found that the addition of Ce in the fuel lowers the activation energy of soot oxidation from about 170 to 120 kJ/mol.

The values of activation energy for catalytic oxidation correspond to dry soot oxidation for samples where the VOF content varies in the range between 2 and 10 per cent.

Keeping constant the above values of activation energy, a certain amount of tuning of the frequency factors, $A$, was allowed. Firstly, the thermal carbon oxidation frequency factors were tuned to represent the experimentally determined thermal regeneration behaviour of the filter (Fig. 5). The catalytic regeneration kinetics (frequency factors) were tuned subsequently to represent the experimentally determined, low-temperature (catalytic) regeneration behaviour of the filter (Fig. 6).

The tuning of the frequency factor values assumes that catalytic regeneration prevails in the temperature range from 400 to 550 °C. Thermal regeneration is more active than catalytic regeneration at higher temperatures. This situation is schematically presented in Fig. 4 by means of comparison between the calculated thermal and catalytic reaction rates as a function of temperature. As can be seen, for the case of catalytic regeneration, the reaction of soot oxidation by CeO$_2$ to CO$_2$ is assumed to be more active after a temperature of 500 °C. This assumption is in accordance with previous experimental work by the present authors that indicates an ignition temperature for the catalytic soot oxidation of the order of 500 °C. Following the same reasoning in the case of thermal regeneration, it may be assumed that the reaction of soot oxidation by exhaust gas oxygen to CO$_2$ is more active above 630 °C where the ignition temperature for thermal oxidation is observed.

After tuning of the model is completed, the ability of the tuned model to predict the effects of additive concentration in fuel, initial soot loading mass, volatile organic fraction of the soot and exhaust mass flowrate was checked.

In principle, the values of the frequency factors should keep close to certain reference values for each reaction of the scheme. However, it must be borne in mind that...
the catalytic reactor in the case of a fuel additive assisted diesel filter is made up of the soot layer, which contains the catalyst dispersed in it, in close contact with the soot. This reactor is destroyed during regeneration and rebuilt during filter loading. The characteristics of the reactor may change according to the prevailing exhaust gas conditions during loading.

The estimated frequency factor values for the catalytic soot oxidation reactions proved sensitive to the ratio of cumulative CO/CO₂ produced during regeneration (Table 4). This indicates the dependence on the filter loading and the regeneration conditions. This observation is confirmed by Aoki et al. [25] and is more pronounced in the case of catalytic regeneration. The assessment of the experimental results showed that the following parameters affect the CO/CO₂ ratio:

1. Soot loading. Increase in soot loading mass over 6 g/l filter causes a significant increase in the CO produced during regeneration.
2. Soot VOF content. Increase in VOF content results in a shift towards higher CO than CO₂ production during regeneration.
3. Exhaust gas mass flowrate. As the exhaust gas mass flowrate increases, more CO than CO₂ is produced during regeneration.

Based on the above reasoning, certain deviations from the reference kinetics of the catalytic reactions are observed in Table 4 and summarized below:

1. It was found that the increase in the initial soot loading shifts the catalytic reaction kinetics to produce more CO and less CO₂. The model can match this behaviour by a respective modification of the frequency factors of the respective reactions.
2. A severe decrease in the volatile organic fraction of the collected particulate leads to a respective reduction in catalytic soot oxidation kinetics, which can be matched by a respective reduction in the frequency factors of the catalytic oxidation reactions.
3. As expected, the tuned one-dimensional model does not successfully predict filter operation at low flowrates. This is due to the importance of complex three-dimensional effects, related to exhaust flow maldistribution and soot loading maldistribution across the filter face.
4. On the other hand, by comparison of model predictions with measurements, it was observed that the catalytic activity is reduced at very high flowrates (very low residence times). This needs to be further investigated.

As regards the pressure drop behaviour, a certain variation in soot permeability was allowed as a function of the following factors:

1. Effect of soot loading. A thicker soot layer leads to a lower permeability–density factor.
2. Effect of the ceria concentration in the fuel. A higher ceria concentration leads to a lower soot permeability–density factor.
3. Effect of VOF. A higher VOF in the soot leads to a lower soot permeability–density factor.

Table 4 presents the wall permeability, soot density and soot permeability times density values inserted in the one-dimensional model to simulate the pressure drop behaviour of the validation experiments.

The measured filter exit temperatures at the central line (measurements taken by thermocouple T/C9) are compared with the predicted ones for each regeneration case in Figs 5 to 13. The correlation observed is satisfactory. However, a certain degree of inaccuracy in predicting the initial heating phase of the regeneration is observed. It is believed that this is a three-dimensional phenomenon related to the change in average mass flowrate owing to the reduction in flow resistance in the central channels [16].

5 DISCUSSION

The comprehensive model presented in this paper is proven able to predict the effect of a significant number
of design and operation parameters on the filter performance in a satisfactory way. In the following, certain important remarks from model validation are discussed in more detail. These remarks generally indicate directions for future, more refined experimental study.

5.1 Catalyst concentration in the fuel

As a first step, the case of regular soot oxidation (no catalyst in the fuel) is studied. The simulation of the regeneration of a filter loaded at 3000 r/min, 40 Nm with the engine operating on regular (not additive doped) fuel is presented in Fig. 5. The values of $E$ determined from TGA experiments produce a satisfactory prediction of the full-scale process in the filter. However, a certain discrepancy between the measured and the predicted filter back pressure is observed in the initial phase of regeneration. As can be seen, the model predicts a slower reduction in the pressure drop as the regeneration initiates. The reason could lie in the fact that this initial phase of the regeneration is associated with a VOF desorption process that is responsible for the rapid back pressure decrease. This situation is not predictable by the one-dimensional pressure drop model, which considers an average soot permeability value during the whole regeneration process.

As a next step, two regeneration experiments with soot collected with 25 and 50 ppm cerium doped fuel were performed. Starting from the simulation of the case with 25 ppm cerium doped fuel described in Fig. 6, it should be mentioned that the fitted value of $(pk)_b$ had to be reduced compared with that for the soot without catalyst. It seems that the presence of catalyst inside the particulate modifies its permeability–density characteristics.

Continuing with the simulation of the case with 50 ppm cerium doped fuel, the results of Fig. 7 indicate that the regeneration behaviour is only a little affected by the higher fuel additive concentration. The effect is that the 50 ppm fuel additive concentration leads to a somewhat lower peak temperature. If the downstream filter CO concentration recordings (not presented in the figures but summarized in Table 4) are examined, it will be seen that the 50 ppm case is associated with somewhat higher CO concentrations (the CO/CO$_2$ ratio is 0.15 as against 0.14 in the 25 ppm case). This hints at the effect, already reported by other researchers [26], of ceria in promoting the CO production. Overall, increase in the catalyst concentration in the fuel from 25 to 50 ppm seems not to produce a higher catalytic effect. On the contrary, the pressure drop behaviour is further affected, and a further decrease in soot permeability is observed. Any attempt to explain these complex effects on the kinetics and pressure drop parameters of soot oxidation by ceria must take into account the in-cylinder particulate formation mechanism which includes the injection and combustion of additive-doped fuel.

![Fig. 7](image_url)

Fig. 7 Simulation of the regeneration of a filter loaded with soot emitted by the engine operating with 50 ppm cerium doped fuel. Measured and predicted trap CO concentration recordings (not presented in the figures) of ceria in observation is confirmed by the results of previous experimental work with single-channel filters [26].

5.2 Initial soot loading

The cases of 3, 6 and 9 g/l filter soot loading were studied. The simulations of the regeneration experiments performed at 2250 r/min, 60 Nm for a filter loaded at 3000 r/min, 40 Nm with the engine operating with 25 ppm doped fuel until the respective loadings are achieved are presented in Figs 8, 6 (reference experiment) and 9. The following trends are observed:

1. From low to medium to high soot mass loading, a decrease in product $(pk)_b$ is observed. Although the increase in soot layer thickness is expected to cause an increase in the soot density owing to layer compression from the exhaust flow, it seems that the decrease in soot permeability is more significant. This observation is confirmed by the results of previous experimental work with single-channel filters [12].

2. As discussed in the previous section, higher frequency factors for catalytic soot oxidation to CO and lower frequency factors for catalytic soot oxidation to CO$_2$ were inserted in the model to match the behaviour with a higher initial soot mass in the filter. The change is more severe for the 9 g/l loading, where, as can be seen in Table 4, the ratio of CO/CO$_2$ becomes about 10 times higher. Any attempt to explain this behaviour must take into account the complex processes of

---


D17503 © IMechE 2004
exhaust gas oxygen diffusion through the soot layer. It could be assumed that, in the initial phase of regeneration, where catalytic soot oxidation prevails over the thermal, the higher soot mass makes more difficult the diffusion of exhaust gas oxygen through the deposit layer, thus preventing the oxidation of CeO$_2$ by O$_2$ to produce CeO$_2$.

5.3 VOF content (soot accumulation condition)

The effects of VOF content on the pressure drop and kinetic parameters could be assessed only indirectly, since the model considers only dry soot oxidation, without separately addressing adsorbed hydrocarbon oxidation by the catalyst. Thus, VOF oxidation kinetics must be lumped in the overall catalytic oxidation kinetics. It is known from the literature that VOF may be oxidized at temperatures as low as 200 °C and also may desorb from the particulate at higher temperatures, or even readsoor at low temperatures. Further improvements by modelling of adsorbed hydrocarbon oxidation are currently in progress, based on a detailed study of the oxidation and sorption behaviour of real diesel particulate produced by modern direct injection (DI) engines when run on catalyst-doped fuel [17]. The two regeneration cases considered in this validation study involve a filter loaded at 3000 r/min, 40 N m (which is a high VOF point) and a filter loaded at 1800 r/min, 90 N m (a low VOF point). The simulations of the regenerations performed at a medium flowrate engine operation point are presented in Figs 6 and 10. Fitting of model parameters to match the experimental behaviour indicates the following trends:

1. From low to high VOF content, a decrease in the value of product $(\rho k)_0$ is observed. It seems that the VOF present in the thick particulate layer reduces the permeability of the soot layer. Furthermore, secondary effects due to the adsorption–desorption processes produced from the temperature differences between the filter core and filter periphery (the VOF preferably condense on the colder outer channels of the filter) may differentiate the permeability characteristics and indicate that the mechanism is three-dimensional.

2. The lower VOF content hints at lower values for the frequency factors of catalytic soot oxidation. This could be attributed to the loss of activity of VOF oxidation which accelerates the dry soot oxidation. According to previous experimental work performed in the LTTE for the investigation of the role of VOF in regeneration behaviour [15], a higher VOF content is associated with a more rapid pressure drop and a higher heat release owing to the higher exothermic nature of HC oxidation. On the other hand, a relative increase in the frequency factor of catalytic soot oxidation to CO$_2$ is necessary in order to match
the decreased CO produced during regeneration (the unburned hydrocarbons are oxidized by ceria mainly to CO).

5.4 Exhaust gas mass flowrate (regeneration condition)

The effect of exhaust gas mass flowrate is studied in four regeneration experiments, conducted with 28, 52, 70 and 92 g/s mass flowrates. The results of the simulations are compared with the measurements in Fig. 6 (52 g/s—reference experiment), Fig. 11 (28 g/s), Fig. 12 (70 g/s) and Fig. 13 (92 g/s). The following trends were observed:

1. The model is capable of predicting the temperature and pressure drop of the filter at medium to high exhaust gas mass flowrate conditions (Figs 6 and 12). The accuracy of the model is reduced at very low or very high mass flowrate conditions (Figs 11 and 13).

2. At low mass flowrate conditions, this is attributed to flow maldistribution phenomena [16]. At such conditions, the point within the filter where the regeneration initiates is stochastic, and the propagation is expected to be slow. The model may not predict this stochastic behaviour because of the assumption of uniform flow distribution at the filter inlet and the assumption of uniform soot mass distribution within the filter. Specifically, in Fig. 11 it may be observed that there is a delay between the computed and the measured temperature in the central channel of the filter, in spite of the fact that the pressure drop during regeneration is well predicted by the model. Moreover, the model also predicts the value of maximum temperature satisfactorily. This indicates that the regeneration did not initiate in the central region of the filter and propagated there with some delay.

3. At medium to high mass flowrates it is expected that the flow inside and at the inlet of the filter becomes more uniform. The assumption of one-dimensional modelling is more realistic at these conditions. This is also supported by the results of Figs 6 and 12, where the computations match the measurements with higher accuracy.

4. Finally, at very high mass flowrates, the amount of CO versus CO₂ at the outlet of the filter because of soot oxidation increases. This is attributed to the lower residence time of exhaust gas within the soot layer because of the higher velocities of the exhaust gas. This effect is not included in the model, and therefore the pre-exponential factor of the thermal soot oxidation to CO had to be increased in order to match the temperature measurement. In addition, the model predicts some regeneration at the beginning of
the measurement owing to the high temperatures of the exhaust gas, although no regeneration occurs. This suggests that, under high exhaust gas temperatures, the catalytic activity diminishes as the flow-rate increases. This may also be connected with the residence time of the exhaust gas in the soot layer, but the phenomenon remains obscure and requires further investigation.

6 CONCLUSIONS

An experimental validation procedure was applied to an improved, comprehensive, one-dimensional model of fuel additive assisted regeneration of a diesel filter. The model features separate consideration of carbon oxidation to CO and CO₂, which enhances its predictive ability. Also, it employs an improved kinetic submodel for the catalytic activity of the cerium-based fuel additive employed.

The validation was based on the results of a number of regeneration tests on the engine bench of a silicon carbide diesel filter fitted to a modern diesel engine run on catalyst (cerium based) doped fuel.

Firstly, the thermal carbon oxidation kinetics (frequency factors) was tuned to represent the experimentally determined thermal regeneration behaviour of the filter.

As a second step, the catalytic regeneration kinetics (frequency factors) were tuned to represent the experimentally determined, low-temperature (catalytic) regeneration behaviour of the filter.

The ability of the tuned model to predict the effects of exhaust mass flowrate, initial soot loading mass, volatile organic fraction of the soot and additive concentration in the fuel was finally checked. The observed deviations from the reference kinetics of the catalytic reactions can be summarized as follows:

1. It was found that the increase in the initial soot loading shifts the catalytic reaction kinetics to produce more CO and less CO₂. The model can match this behaviour by the respective modification of the frequency factors of the respective reactions.

2. A severe decrease in the volatile organic fraction of the collected particulate leads to a respective reduction in the catalytic soot oxidation kinetics, which can be matched by a respective reduction in frequency factors of the catalytic oxidation reactions.

3. As expected, the tuned one-dimensional model does not successfully predict filter operation at low flow-rates. This is due to the importance of complex three-dimensional effects, related to exhaust flow mal-distribution and soot loading mal-distribution across the filter face.

Diagrams:

Fig. 12  Simulation of a medium mass flowrate regeneration scenario (70 g/s). Measured and predicted trap temperatures near the exit of a central channel during a low mass flowrate regeneration performed at 3000 r/min, 60 N m for a medium mass loaded filter at 3000 r/min, 40 N m with 25 ppm Ce doped fuel. Also, measurement and prediction of the filter back pressure together with soot mass prediction are presented. Computation is made with \( (\rho k) = 2.2 \times 10^{-13} \text{ kg/m} \), activation energies \( E_1 = 1.9 \times 10^5 \), \( E_2 = 1.5 \times 10^5 \), \( E_3 = 1.2 \times 10^5 \), \( E_4 = 0.8 \times 10^5 \) and \( E_5 = 0.8 \times 10^5 \) J/mol and frequency factors \( A_1 = 1 \times 10^{13}, A_2 = 5.5 \times 10^{10}, A_3 = 3.5 \times 10^{11}, A_4 = 6 \times 10^8 \) and \( A_5 = 8 \times 10^9 \) mol/m³ s.

Fig. 13  Simulation of a high mass flowrate/high-temperature regeneration scenario (100 g/s). Measured and predicted trap temperatures near the exit of a central channel during a high mass flowrate regeneration performed at 4000 r/min, 40 N m for a medium mass loaded filter at 3000 r/min, 40 N m with 25 ppm Ce doped fuel. Also, measurement and prediction of the filter back pressure together with soot mass prediction are presented. Computation is made with \( (\rho k) = 2.2 \times 10^{-13} \text{ kg/m} \), activation energies \( E_1 = 1.9 \times 10^5 \), \( E_2 = 1.5 \times 10^5 \), \( E_3 = 1.2 \times 10^5 \), \( E_4 = 0.8 \times 10^5 \) and \( E_5 = 0.8 \times 10^5 \) J/mol and frequency factors \( A_1 = 1 \times 10^{13}, A_2 = 6.5 \times 10^{10}, A_3 = 3.5 \times 10^{11}, A_4 = 6 \times 10^8 \) and \( A_5 = 8 \times 10^9 \) mol/m³ s.
4. On the other hand, by comparison of model predictions with measurements, it was observed that the catalytic activity is reduced at very high flowrates (very low residence times). This needs to be further investigated.

Along with the validation of the kinetic submodel, a validation of the pressure drop submodel was carried out.

The results of the validation procedure are intended to demonstrate the scope and extent of applicability of the specific model category to real-world design and optimization studies with diesel filters.

REFERENCES


10 Tan, J. C., Opris, C. N., Baumgard, K. J. and Johnson, J. H. A study of the regeneration process in diesel particulate traps using a copper fuel additive. SAE paper 960136, 1996.


26 de Soete, G. Catalysis of soot combustion by metal oxides. In Western States Section Meeting: The Combustion Institute, Salt Lake City, 21–22 March 1988.